Stochastic Hybrid Models and Algorithms for Fluids Highlight Fluctuating Hydrodynamics for Reaction-Diffusion Systems

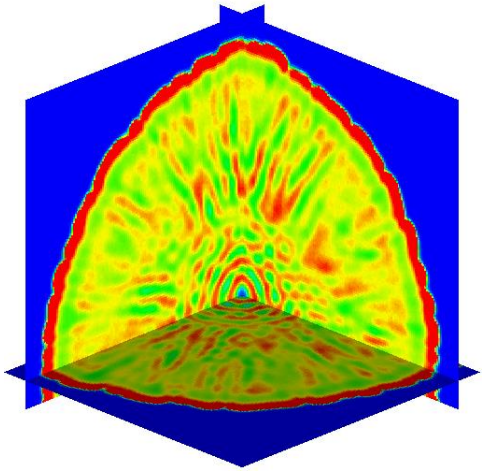
Objectives

- Develop a new stochastic simulation methodology for reaction-diffusion problems
- Combine the rigor of the master equation approach for reactions and the efficiency of the fluctuating hydrodynamics approach for diffusion
- Construct a numerical method that scales well for increasing number of molecules and also is robust to handle trace reactive species

Impact

- Enable efficient stochastic simulation of large-scale and high-dimensional reaction-diffusion problems
- Provide predictive capability relevant to a number of fields, including: cell biology and nanoparticle synthesis
- Provide a framework for the inclusion of accurate description of reactions into general fluctuating hydrodynamic equations

Three-dimensional chemical front propagation involving the equivalent of 10^{12} molecules



Accomplishments

- Developed efficient and robust numerical methods for reaction-diffusion problems
- Verified that our methods faithfully reproduce results from the traditional reaction-diffusion master equation approach with remarkable computational efficiency
- Demonstrated the importance of thermodynamic fluctuations to the Turing-like pattern formation and chemical front propagation

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